

Quasi-particle spectrum around a single vortex in s -wave superconductors

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Abstract

Making use of the Bogoliubov-de Gennes equation, we study the quasi-particle spectrum and the vortex core structure of a single vortex in quasi 2D s -wave superconductors for small $p_F\xi_0$, where p_F is the Fermi momentum and $\xi_0 = v_F/\Delta_0$ is the coherence length ($\hbar = 1$). In particular we find that the number of bound states decreases rapidly for decreasing $p_F\xi_0$. Also for $p_F\xi_0 \sim 1$, the Kramer-Pesch effect stops around $T/T_c \simeq 0.3$.

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I. INTRODUCTION

There are renewed interest in the vortex structure since the discovery of the high T_c cuprate superconductors. Perhaps the superconductivity of high T_c cuprates is characterized as d -wave superconductivity^{1,2} and is very close to the quantum limit^{3,4}.

Schopohl and Maki have studied earlier the quasi-particle spectrum around a single vortex line in terms of quasi-classical equation^{5,6} and predicted a clear four fold symmetry for a d -wave superconductor⁷. Then a beautiful STM study of vortices in YBCO monocrystals was reported⁸. A big surprise is first of all the quasi-particle spectrum exhibits a circular symmetry. There is no trace of four-fold symmetry. Second, there appears to be only a single bound state with energy $\approx \frac{1}{4}\Delta(0)$ where $\Delta(0)$ ($= 260\text{K}$) is the superconducting order parameter at $T = 0\text{K}$. A similar bound state energy is observed earlier by a far-infrared magneto-transmission from YBCO film by Karraï *et al.*⁹. If you recall the analysis of bound states around the vortex core by Caroli and co-workers¹⁰, there should be thousands of bound states. Of course in usual s -wave superconductors we have $p_F\xi_0 \approx 10^3 \sim 10^4$, where p_F is the Fermi momentum and $\xi_0 = v_F/\Delta(0)$ is the coherence length ($\hbar = 1$). So perhaps the single bound state in YBCO suggests³ $p_F\xi_0 \approx 1$. At the first sight this suggestion looked outrageous, since this implies $E_F \approx 200 \sim 500\text{K}$ in YBCO. By analyzing the spin gap at $T = 0\text{K}$ observed in YBCO monocrystals by inelastic neutron scattering by Rossat-Mignod *et al.*¹¹, we can deduce the chemical potential μ given as¹²,

$$\mu = -345(x - 0.45)\text{K} \quad (1)$$

where x is the oxygen dopage corresponding to $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$. Then for optimally doped YBCO we obtain $\mu = -190\text{K}$.

In Döttinger *et al.*⁴ the flux flow resistance of 60 K YBCO measured by Matsuda *et al.*¹³ is analyzed and they identified the Kramer-Pesch effect characteristic to the superconductor in the clean limit^{14,15}. On the other hand apparently the Kramer-Pesch effect is absent in 90 K YBCO¹³, implying again perhaps 90 K YBCO is in the quantum limit⁴. Here Kramer-Pesch effect means that the vortex core shrinks with decreasing temperature due to the decrease in the occupied bound states around the vortex line. The core size is expressed as¹⁴

$$\xi_1 = \frac{v_F}{\Delta(T)} \frac{T}{T_c}. \quad (2)$$

This reduction of the core size results to the nonlinear conductivity^{4,15}. Ichioka *et al.*¹⁶ found the Kramer-Pesch effect in d -wave superconductivity with the help of the semi-classical approach developed in Ref. 7.

But if $p_F\xi_0 \approx 1$, this implies the semi-classical approach introduced in Ref. 5 and Ref. 6 is no longer reliable in studying the vortex in the high T_c cuprates. So Morita, Kohmoto and Maki¹⁷ studied Bogoliubov-de Gennes equation for a single vortex in d -wave superconductors. Indeed choosing $p_F\xi_0 = 1.33$, they can describe gross features of STM result for YBCO. On the other hand they have not attempted the self-consistency due to the numerical difficulties. Nevertheless they discovered there is a single bound state for $p_F\xi_0 = 1.33$ in the vortex of d -wave superconductors. Further there are low energy ($E \leq 0.1\Delta$) extended states with four legs stretched in the four diagonal directions $(1, 1, 0)$ and $(1, -1, 0)$. Recently these extended states are rediscovered by Franz and Tešanović¹⁸ in a model somewhat different

from the one in Ref. 17. Also in the model of Franz and Tešanović they don't have any bound state. But since they introduced a large short range Coulomb repulsion, it is very likely the bound state is completely knocked off.

In order to avoid the mathematical complication related to d -wave superconductors and to prepare for such a study in d -wave superconductors, we study in this paper the quantum limit of a single vortex in s -wave superconductors. Contrary to d -wave superconductors the angular momentum around the vortex is a good quantum number, which simplifies the problem. Indeed we can follow the formalism set up in Gygi and Schlüter¹⁹ except we are now interested in the region of small $p_F\xi_0$. Recently a related study by Hayashi *et al.*²⁰ is reported. Unfortunately they have used the $p_F\xi_0$ dependent cutoff energy rather than the constant cutoff energy. So the comparison of systems with different $p_F\xi_0$ appears to have involved some artifact. One of our purposes is to find the result free from artifact.

In the following we limit ourselves to $p_F\xi_0 = 1, 2$ and 4 and study the quasi-particle spectrum and the shape of $|\Delta(r)|$ as a function of temperature. Even for $p_F\xi_0 = 1$ we find 3 bound states at $T = 0\text{K}$. Also the Kramer-Pesch effect which is present at $T/T_c \simeq 0.5$ appears to stop at $T/T_c = 0.3$ for $p_F\xi_0 = 1$. Finally the shape of $|\Delta(r)|$ appears to depend crucially on the $u_0(r)v_0^*(r)$, where $u_0(r)$ and $v_0(r)$ are the wave function associated with the lowest bound state energy. We also show the local quasi particle density of states which exhibits remarkable structures.

II. BOGOLIUBOV-DE GENNES EQUATION

The spatial dependence of order parameters of the superconductivity is described by the Bogoliubov-de Gennes equation. We consider the case with low magnetic field near H_{c1} so that there is a single vortex. Therefore we can ignore the vector potential. In this case the Bogoliubov-de Gennes equation becomes

$$\left(-\frac{1}{2m_e}\nabla^2 - \mu\right)u_n(\mathbf{r}) + \Delta(\mathbf{r})v_n(\mathbf{r}) = E_n u_n(\mathbf{r}), \quad (3a)$$

$$-\left(-\frac{1}{2m_e}\nabla^2 - \mu\right)v_n(\mathbf{r}) + \Delta^*(\mathbf{r})u_n(\mathbf{r}) = E_n v_n(\mathbf{r}), \quad (3b)$$

where $u_n(\mathbf{r})$ and $v_n(\mathbf{r})$ are quasi-particle wave functions.

We take z -axis along to the vortex line. We consider nearly two-dimensional case for simplicity, where kinetic term associated to the z direction is negligible. In the following, we merely consider two-dimensional case and we take a cylindrical coordinate. Taking the gauge as $\Delta(\mathbf{r}) = |\Delta(r)|e^{-i\theta}$, angular momentum of each eigenstate becomes half odd integer $m + \frac{1}{2}$. Then $u_n(\mathbf{r})$ and $v_n(\mathbf{r})$ becomes as follows,

$$u_n(r, \theta) = u_{nm}(r) \frac{e^{im\theta}}{\sqrt{2\pi}}, \quad (4a)$$

$$v_n(r, \theta) = v_{nm}(r) \frac{e^{i(m+1)\theta}}{\sqrt{2\pi}}. \quad (4b)$$

Following Gygi and Schlüter¹⁹, we apply Fourier-Bessel expansion with basis;

$$\phi_{mj}(r) = \frac{\sqrt{2}}{RJ_{m+1}(\alpha_{jm})} J_m(\alpha_{jm} \frac{r}{R}) \quad (5)$$

to $u_{nm}(r)$ and $v_{nm}(r)$, where α_{jm} is j -th positive zero of the Bessel function of m -th order $J_m(x)$. Then wave functions become as,

$$u_{nm}(r) = \sum_j u_{nmj} \phi_{mj}(r), \quad (6a)$$

$$v_{nm}(r) = \sum_j v_{nmj} \phi_{m+1j}(r). \quad (6b)$$

$$(6c)$$

Here, the boundary condition is such that wave functions are zero at the edge of the disk with radius R . Then the Bogoliubov-de Gennes equation becomes,

$$\left[\frac{1}{2m_e} \left(\frac{\alpha_{jm}}{R} \right)^2 - \mu \right] u_{nmj} + \sum_{j_1} \Delta_{jj_1} v_{nmj_1} = E_{nm} u_{nmj}, \quad (7a)$$

$$- \left[\frac{1}{2m_e} \left(\frac{\alpha_{j, m+1}}{R} \right)^2 - \mu \right] v_{nmj} + \sum_{j_1} \Delta_{j_1j} u_{nmj_1} = E_{nm} v_{nmj}, \quad (7b)$$

where $\Delta_{j_1j_2}$ is given as,

$$\Delta_{j_1j_2} = \int_0^R \phi_{mj_1}(r) |\Delta(r)| \phi_{m+1j_2}(r) r dr. \quad (8)$$

The order parameter is given as,

$$|\Delta(r)| = g \sum_{|E_n| \leq E_c} \sum_{m \geq 0} \sum_{j_1 j_2} u_{nmj_1} v_{nmj_2} \phi_{mj_1}(r) \phi_{m+1j_2}(r) [1 - 2f(E_{nm})], \quad (9)$$

where g is the interaction constant, E_c is the cutoff energy and $f(E)$ is the Fermi distribution function. We solve these equations self-consistently. We fix the cutoff energy ($E_c = 5\Delta_0$ for the case of largest Fermi momentum) and the interaction constant, and choose the Fermi momentum p_F so that $p_F \xi_0 = 1, 2$ and 4 .

III. RESULTS

In the numerical calculation, the radius of boundary is taken as $R = 10\xi_0$ and maximum angular momentum and number of zero points of Bessel functions are taken so that all of the quasi-particle states within cut-off energy are taken into the calculation.

A. temperature dependence of order parameter

The temperature dependence of the order parameter is shown in Fig.1. Near the boundary $r/\xi_0 = 10$, the order parameter goes to zero and there is a peak before that. These are effects from the boundary condition and the finite size. But core structures are not affected by the boundary condition.

For $p_F\xi_0 = 4$ at low temperature ($T/T_c \leq 0.1$) there is a shoulder in $|\Delta(r)|$ at the vortex core. This feature comes from bound states in the vortex core. This can be seen from Fig.2, where contributions of the scattering states and the bound states are shown separately. For $p_F\xi_0 = 1$, the peak position of the contribution to the order parameter is located slightly outside of vortex core. Therefore the core structure is not so much affected by the bound states. For larger $p_F\xi_0$ (~ 16), Hayashi *et al.*²⁰ showed the oscillation of the order parameter at the inside of the vortex core. It appears that the origin of this oscillation is the reflection of the bound state wave functions contrary to their interpretation.

Slightly increasing temperature, the bound state contribution decreases rapidly and scattering state contribution remains almost the same. In this temperature range, the core size is dominated by the bound states. Above this temperature region, scattering state contribution decreases with increasing temperature as the behavior of the order parameter of the uniform solution.

We also plot the quasi particle wave function $u_{n\mu}(r)$ and $v_{n\mu}(r)$ of three bound states for $p_F\xi_0 = 4$ in Fig.3. From these figures, it can be seen that main contribution to the core structure comes from the lowest energy bound state. Also we can see $u(r)$ of the lowest energy bound state behaves like s -wave function and $v(r)$ behaves like p -wave function. Similar behavior also can be seen for second and third lowest bound states. They belong to the angular momentum m and $m + 1$ state respectively.

B. Quasi-particle spectrum

In Fig.4 we give quasi-particle energies with angular momentum $m + \frac{1}{2}$ and we also plot those of the uniform state in order to compare the vortex state and the uniform state. For small angular momentum, lowest energy states become bound states lowering its energy and slightly increasing energies of higher energy states. For larger angular momentum, the quasi-particle energy is almost same for vortex and uniform states and there is no bound state. Although it is difficult to say the boundary of these two cases in the angular momentum, the number of bound states may be counted as 20 for $p_F\xi_0 = 4$, 7 for $p_F\xi_0 = 2$ and 3 for $p_F\xi_0 = 1$. The temperature dependence of quasi-particle energy is shown in Fig.5. In this figure we plot quasi-particle energies of the several bound states normalized with the order parameter $\Delta(T)$ at $r = 5.5\xi_0$. From this figure we can see that for smaller $p_F\xi_0$ and higher energy states, the quasi-particle energy varies parallel to the order parameter with temperature. But lower energy states for larger $p_F\xi_0$, the quasi-particle energy increases rapidly with decreasing temperature and becomes constant at low temperature. This behavior of the energy of the lowest bound state was already noted by Gygi and Schlüter¹⁹ for much larger $p_F\xi_0$ but the energy increases with decreasing temperature even at low temperature because of the large $p_F\xi_0$.

C. Core radius

As mentioned in III A, the core structure depend on the bound states. As defined by Kramer and Pesch¹⁴, we calculate core radius ξ_1 as

$$\frac{1}{\xi_1} = \lim_{r \rightarrow 0} \frac{\Delta(r)}{r\Delta_0}, \quad (10a)$$

$$= \frac{g}{\Delta_0} \sum_{E_{nm} \leq E_c} \sum_{j_1 j_2} u_{n0j_1} v_{n0j_2} [1 - 2f(E_{n0})] \phi_{j_1 0}(0) \frac{d\phi_{j_2 1}}{dr}(0). \quad (10b)$$

We plot total ξ_1^{-1} and a contribution from scattering states to ξ_1^{-1} in Fig.6. The temperature dependence of ξ_1 is almost linear in the intermediate temperature region according to Kramer and Pesch¹⁴. For $p_F \xi_0 = 4$, there is a substantial decrease of the core radius at low temperature because of empty bound states. Although for smaller $p_F \xi_0$ there is a bound state contribution, its peak position of the contribution to the order parameter is nearly at the edge of the core. Therefore the core radius is not much affected. But for large $p_F \xi_0$, the peak of the contribution of the bound states are well inside of the core, so the core radius shrinks significantly.

Comparing with Fig.5 in Ref. 19, our result for small $p_F \xi_0$ shows saturations of ξ_1^{-1} at $T/T_c \approx 0.1$ for $p_F \xi_0 = 4$, $T/T_c \approx 0.2$ for $p_F \xi_0 = 2$ and $T/T_c \approx 0.3$ for $p_F \xi_0 = 1$. This comes from finiteness of the bound states.

D. Current density and magnetic field

Current density is calculated from

$$\mathbf{j}(\mathbf{r}) = \frac{e}{2m_e i} \sum_{nm} \{f(E_{nm}) u_{nm}^*(\mathbf{r}) \nabla u_{nm}(\mathbf{r}) + [1 - f(E_{nm})] v_{nm}(\mathbf{r}) \nabla v_{nm}^*(\mathbf{r}) - \text{h.c.}\}. \quad (11)$$

There is a rotational symmetry, so the current has only θ component;

$$j_\theta(r) = \frac{e}{m_e} \sum_{nm} \left\{ f(E_{nm}) \frac{m}{r} |u_{nm}(r)|^2 - [1 - f(E_{nm})] \frac{m+1}{r} |v_{nm}(r)|^2 \right\}. \quad (12)$$

We show this current density at $T = 0.1T_c$ in Fig.7 for each $p_F \xi_0$. The peak position of the current density is same as the peak position of the lowest energy bound state. Therefore smaller $p_F \xi_0$ the peak is located further from the vortex core. Therefore there is no simple relation between the core size and the peak position of the current.

From Maxwell equation, we calculate magnetic field parallel to the z -axis as,

$$H_z(r) = \frac{4\pi}{c} \int_r^R j_\theta(r) dr, \quad (13)$$

and we normalized it with $\phi_0/2\pi\lambda^2$ and show in Fig.8, where $\lambda = (m_e c^2/4\pi n e^2)^{1/2}$ is the penetration depth and $\phi_0 = hc/2e$ is the flux quantum. From this figure, we find that for smaller $p_F \xi_0$ the distribution of magnetic field is more extended to outside of the vortex core.

E. Local density of states

In order to compare with the STM experiments, we calculate the local density of states with thermal average,

$$N(r, E) = \sum_{nm} \{ |u_{nm}(r)|^2 f'(E_{nm} - E) + |v_{nm}(r)|^2 f'(E_{nm} + E) \}. \quad (14)$$

We also take spatial average with a Gaussian distribution with standard deviation $0.1\xi_0$. This is shown in Fig.9. In this figure there is a oscillation at $E/\Delta_0 > 1.0$, where Δ_0 is the average value of the order parameter at the outside of the vortex core. This feature comes from the finite size of our system and it is an artifact.

In addition to this, there are several peaks due to the discrete bound states for energy less than the energy gap ($E < \Delta_0$) and there is a particle-hole asymmetry in contrast to the result of Gygi and Schlüter¹⁹. Wang and MacDonald²¹ showed this asymmetry by solving lattice model and also Morita *et al.*¹⁷ and Hayasi *et al.*²⁰ pointed out it previously. For smaller $p_F\xi_0$, this discrete structure is more apparent.

IV. CONCLUSION

In summary, we have solved the Bogoliubov-de Gennes equation for a single vortex state in s-wave superconductors for small $p_F\xi_0$ and obtain the electronic structure around the vortex core. We show the effect of the discrete bound states to the order parameter structure, the local density of states, the current density and the magnetic field. For smaller $p_F\xi_0$, the contribution of the bound state decreases and depends on the peak positions of wave functions of quasi particles. Also the discreteness of the bound states is more apparent for smaller $p_F\xi_0$.

Recently Sonier *et al.*²² claimed that they obtained the core size of the vortex in NbSe₂ by measuring the peak position of the current density. But there are a few problems in their procedure. First, as we have shown there is no simple relation between the core size and the peak in the current density. Second even if such a relation exists the relation between these quantities are different in the clean limit from the dirty limit result shown in Ref. 22. In particular the core size in the clean limit is much smaller than the one in the dirty limit with respect to the peak position in the current density. At least they should have analyzed their data in the light of the clean limit calculation by Gygi and Schlüter¹⁹.

Our calculation has been done on the s-wave superconductivity in the quantum limit. For high T_c cuprates, d-wave superconductivity is required. Also in the quantum limit, the effects from the constraint of the number conservation may be large as pointed by van der Marel²³, although we have fixed $p_F\xi_0$ for all temperature region. Therefore, the anisotropy of the superconductivity and the constraint of the number conservation must be taken into account in the study of the vortex in high T_c cuprates. These are left as future problems.

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FIGURES

FIG. 1. The temperature dependence of the order parameter $\Delta(r)$ for $p_F\xi_0 = 4$ (a), $p_F\xi_0 = 2$ (b) and $p_F\xi_0 = 1$ (c). The order parameter is normalized with $\Delta_0 = \Delta(r = 5.5\xi_0, T = 0)$ for each $p_F\xi_0$.

FIG. 2. Contributions from the bound states and the scattering states to the order parameter for $p_F\xi_0 = 4$ (a), $p_F\xi_0 = 2$ (b) and $p_F\xi_0 = 1$ (c), where $\Delta_0 = \Delta(r = 5.5\xi_0, T = 0)$.

FIG. 3. The quasi particle wave functions $u(r)$ and $v(r)$ and their product with thermal factor for the first (a), the second (b) and the third (c) of the lowest energy bound states.

FIG. 4. The quasi particle spectrum of the vortex state(\diamond) and the uniform state(dashed line) for $p_F\xi_0 = 4$ (a), $p_F\xi_0 = 2$ (b) and $p_F\xi_0 = 1$ (c).

FIG. 5. The temperature dependence of the quasi-particle energies of the bound states in the vortex state. The energies are normalized by the order parameter $\Delta(T)$ at $r/\xi_0 = 5.5$. (a), (b) and (c) are for $p_F\xi_0 = 4$, $p_F\xi_0 = 2$ and $p_F\xi_0 = 1$, respectively

FIG. 6. The temperature dependence of ξ_1^{-1} for $p_F\xi_0 = 1, 2$ and 4. Also contributions from scattering states for each $p_F\xi_0$ are plotted.

FIG. 7. The current density at $T = 0.1T_c$ for $p_F\xi_0 = 4$ (a), $p_F\xi_0 = 2$ (b) and $p_F\xi_0 = 1$ (c). The current density is normalized with its maximum value. The order parameter is also shown for comparison.

FIG. 8. The spatial dependence of the magnetic field H at $T = 0.1T_c$ for $p_F\xi_0 = 1, 2$ and 4.

FIG. 9. The local density of states $N(r, E)$ at $T/T_c = 0.1$ for $p_F\xi_0 = 4$ (a), $p_F\xi_0 = 2$ (b) and $p_F\xi_0 = 1$ (c). $N(r, E)$ is normalized with the density of states of the normal state N_0 .

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